

1-Propanol-1,1-d2
40422-04-6 | DTXSID30480194

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 13.1 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.76e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

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1-Propanol

Measured: 16.6

Predicted: 13.1

Image not found

Isopropanol

Measured: 16.6

Predicted: 9.46

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But-2-en-1-ol

Measured: 13.9

Predicted: 6.02

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Allyl alcohol

Measured: 17.2

Predicted: 14.2

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Methallyl alcohol

Measured: 2.69

Predicted: 6.51